Resonance-hybridization version of the Mott transition

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It is shown on the basis of a model material, p-CdSnAs$_2\langle$Cu$\rangle$, that a superposition of localized impurity-band states on the band continuum causes a resonance-hybridization version of the Mott transition through the impurity band. In the course of this transition, the mobility of the impurity-band carriers is "pulled" toward the mobility of the band carriers.

A point which remains unresolved in semiconductor physics is the nature of the conductivity through a resonant impurity band with anomalously high carrier mobilities.[1,2] Other problems which have not been studied concern how a hybridization of the states of the band continuum with states of the resonant impurity band affects the dynamics of the metal–insulator transition and the structure of the tail on the density of states of the band of a heavily doped semiconductor.

A convenient model material for corresponding research is[3] p-CdSnAs$_2\langle$Cu$\rangle$. The tail of the conduction band of this material has a deep acceptor band, at a distance $\epsilon_A = (-30 + 4.6\times 10^2\ \mathrm{T} - 120\ \mathrm{P})\,\mathrm{meV}$ (where T is in kelvins, and P in gigapascals) from the unperturbed edge of the conduction band. The acceptor band is linked with the valence band in terms of energy. Consequently, with increasing hydrostatic pressure, the conduction band moves away from these bands at the same rate.

We carried out experiments on heavily doped and strongly compensated crystals, which were subjected to hydrostatic compression at pressures up to $P = 1.5$ GPa, at $T = 2$–300 K and in magnetic fields up to $H = 15$ kOe. We measured the Hall coefficient $R(T,P,H)$ and the conductivity $\sigma(T,P)$. The Hall coefficient at a fixed temperature increases with increasing P and H, going from negative values to positive values. In the limit $P, H \to \infty$, it tends toward $R_\infty = (N_\infty e)^{-1}$, where N_∞ is the concentration of excess acceptors. Since we have $R > 0$ at $T = 77.6$ K, even at atmospheric pressure, we have $p/n > (\mu_e/\mu_A)^2 \gg 1$, where n and p are the densities, and μ_e and μ_A the mobilities, of electrons and holes, respectively. Consequently, the partial values corresponding to the acceptor band are $\sigma_A \simeq \sigma$, $R_A \simeq R_\infty$ and $p = N_\infty \gg n$ (p does not depend on T or P), and we have $\mu_\mathrm{A} \simeq \mathrm{R}_\infty \sigma$. In other words, at $T < 77.6$ K the quantity $\sigma(T,P)$ differs from $\mu_A(T,P)$ by a constant numerical factor R_∞. Looking at μ_e at a fixed P, we see that it differs by a constant numerical factor of $R_e = (ne)^{-1}$ from $\sigma_e(T)$ at $T < 40$ K. From the data on R and σ we calculate n, p, μ_e, μ_A, using the two-band model and assuming a constant relaxation time.[1–4]

The results of the analysis of the experimental data are shown in Figs. 1–3. It can be seen from Figs. 1 and 2 that near atmospheric pressure we observe a simultaneous transition of conduction-band electrons and acceptor-band holes from a nonactivated metallic conductivity to a Mott hopping conductivity: $\mu_{e,A} \sim \exp\{(-T_{oe,A}/T)^{1/4}\}$.

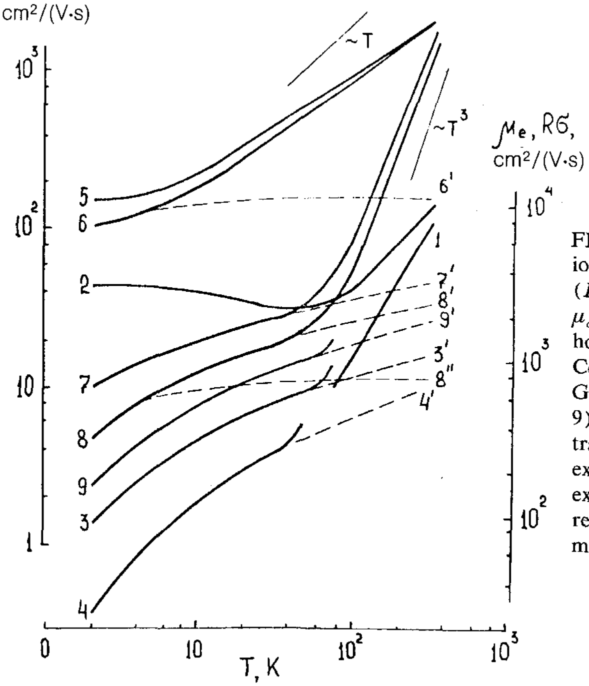

FIG. 1. Temperature dependence of various properties. 1—The Hall mobility $R\sigma$ ($H = 15$ keV); 2–4—the electron mobility μ_e; 5–9—the mobility of acceptor-band holes, μ_A, in sample 14D-1 of *p*-CdSnAs$_2$⟨Cu⟩. The pressure P is: 5) 10^{-4} GPa; 1,2,6) 0.02; 3,7) 0.42; 8) 1.14 GPa; 9) $P \to \infty$. Lines 3′, 4′, and 6′–9′ are extrapolations of the Mott law; line 8″ is an extrapolation of the dependence $\exp(-\epsilon_3/kT)$ out of the low-temperature region (2–5 K). The solid lines are experimental.

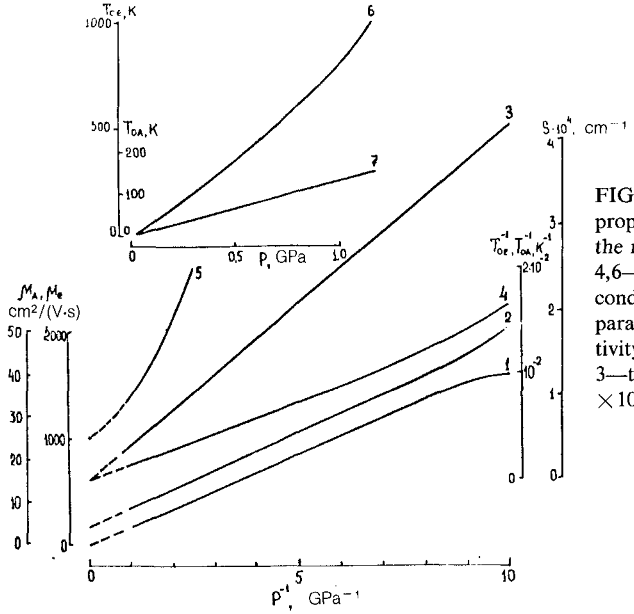

FIG. 2. Pressure dependence of several properties. 1—The electron mobility; 2—the mobility of acceptor-band holes, μ_A; 4,6—the parameter of the Mott hopping conductivity of electrons, T_{oe}; 5,7—the parameter of the Mott hopping conductivity of the acceptor-band holes, T_{oA}; 3—the parameter $S = (n^{-1/3} - 7.75 \times 10^{-5})^{-1}$ (at 4.2 K in sample 14D-1).

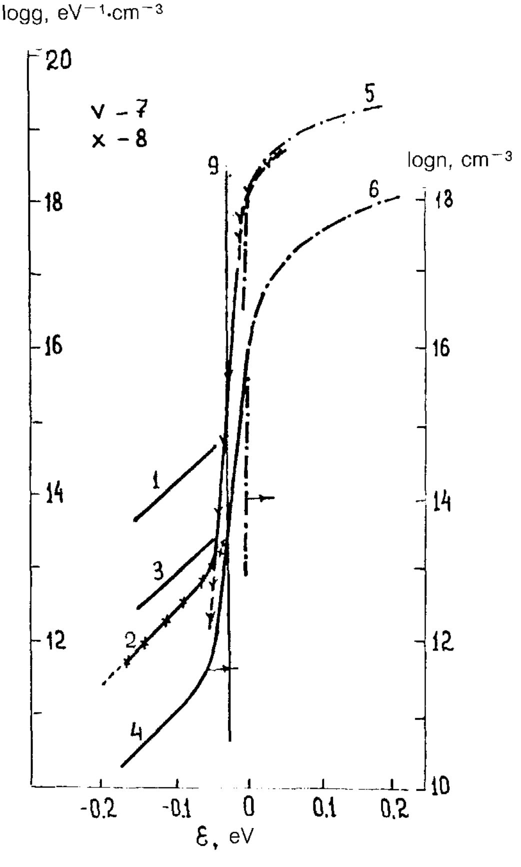

FIG. 3. Energy dependence of various properties. 1,2—Density of states of the conduction band; 3,4—the electron density [at 4.2 K; sample 15D-2 (1 and 3) and sample 14D-1 (2 and 4) of p-CdSnAs$_2$⟨Cu⟩]. The origin of the energy scale corresponds to the unperturbed edge of the conduction band. Solid lines: Experimental. Dot–dashed lines: Density of states (5) and electron density (6) of ideal CdSnAs$_2$. Dashed line and points (7): Semiclassical theory of linear screening[4] for $\gamma = 14.8$ meV. Dashed line and points (8): The approximation $g_e = 2.55 \times 10^{12} \cdot \chi^{-3/2} \exp(-x^2)$, where $\chi = |\epsilon|/\gamma$, and $\gamma = 145.3$ meV. (9): Density of states of the acceptor band.

With increasing P, the parameters $T_{oe,A}$ increase from the zero value corresponding to the boundary of the metal–insulator transition. In the limit $P \to \infty$ we have $T_{oe} \to \infty$ ($\mu_e \to 0$). The quantities of T_{oA} and μ_A tend toward fixed values (Fig. 2), as follows from the energy dependence of the density of states (Fig. 3). On the tail of the density of states of the conduction-band electrons we can distinguish two regions (Fig. 3). Near the edge of the conduction band, between $\epsilon = 0$ and -50 meV, we have $g_e = 1.5 \times 10^{18} \exp(0.22\epsilon_A)$, and n decreases sharply, by 4 or 5 orders of magnitude. Actually, this is the deformed edge of the conduction band (deformed by the random potential). Deep in the tail of the density of states, between -50 and -170 meV, we have $g_e = 2.3 \times 10^{13} \exp(0.023\epsilon_A)$. It also follows from the experimental data (Figs. 1–3) that the energy of the percolation level of the electrons of ϵ_1 conductivity (ϵ^1_{pe}) coincides with the energies ϵ_F and ϵ_A near atmospheric pressure, where we have $T_{oe,A} = 0$ i.e., $\epsilon^1_{pe} = \epsilon^0_F \epsilon^0_A = -30$ meV. The critical density of electrons is $n_{cr} = 10^{13}$ cm^{-3}. If n_{cr} is known, we can use the expression[4] $n_{cr} = \beta N_i^{2/3}/a_{Be}$ (N_i is the total impurity concentration, and a_{Be} is the electron Bohr radius) to determine the previously unknown numerical factor β: $\beta = 10^{-5}$. It follows from the expression for the average value of the random potential,[4] $\gamma = \nu_1 e^2 N_i^{2/3}/(\chi n^{1/3})$ (χ is the dielectric constant), and from the relation $\gamma = |\epsilon_F = |\epsilon_A| = |\epsilon^0_A - 120P|$ that we have $\nu_1 = 1.85 \times 10^{-2}$ and $\epsilon^0_A = -37$ meV. This result agrees with the value found in Ref. 3. No theoretical prediction of the coefficient ν_1 is available.

Up to a pressure of 1.8 GPa, under the condition $\gamma < 0.5\epsilon_g$ (ϵ_g is the width of the band gap), i.e., before we reach the situation corresponding to the model of a fully compensated semiconductor,[4] the Fermi level is rigidly pinned in the acceptor band, which acts as an electron reservoir. The role played by the pressure reduces to one of scanning the Fermi level in the tail of the density of states of the conduction band and thinning out the band states. As a result, electrons localize at fluctuational wells of the impurity potential (a semiclassical version of an Anderson transition), and holes also localize. The holes are delocalized by a resonance of the acceptor band states and the conduction-band states and by their hybridization. Consequently, the transition is a resonance-hybridization version of the Mott transition in this case, and it proceeds until a limiting impurity concentration is reached. A characteristic feature of the resonance-hybridization version of the Mott transition is a resonant "pulling" of the mobility of the impurity-band carriers toward the mobility of the band carriers. This pulling intensifies with increasing T (Fig. 1). At this point it is useful to make a comparison with resonant scattering.[2] Resonant scattering is responsible for the decrease in the ratio μ_e/μ_A with decreasing P near the transition (Fig. 2; see also Ref. 3) and the high values of the carrier mobility of the resonant impurity band.[1,2] The limiting case ($\mu_e/\mu_A = 1$) is observed in narrow-band, heavily doped semiconductors like n-InSb, in which a resonance-hybridization version of the Mott transition occurs until a limiting impurity concentration is reached.

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